COBLENTZ SOCIETY NEWSLETTER

Mailing No. 35 August 15, 1967

I. Coblentz Society Symposium

For the benefit of those members who were unable to attend the 1967 Coblentz Symposium at Pittsburgh on "Where Does Infrared Spectroscopy Go from Here?", we enclose an account of the session reprinted from Scientific Research. Several papers are not represented in this account; a summary of one of them is appended.

II. Coblentz Award

The award committee is soliciting nominations for the 1968 Coblentz Award. The award is made on the basis of the candidate's published research in the field of molecular spectroscopy applied to the elucidation of chemical problems. The prize winner must not have passed his 36th birthday by December 31st of this year. Men and women are equally eligible; there are no geographical restrictions; and membership in the Coblentz Society is not a prerequisite. If you have a candidate in mind, please send his or her name to Dr. H. B. Kessler, Secretary, The Coblentz Society, 761 Main Avenue, Norwalk, Connecticut 06851, before October 1st.

III. Infrared Techniques Abstracts

Two issues of abstracts have now been published (Mailings 33 and 34). Dr. Leopold May, who has been compiling them, would like an indication as to whether or not this feature is useful to the membership. If you have an opinion on this matter, please write a note either to the editor of this newsletter or to Dr. May; Department of Chemistry, The Catholic University of America, Washington, D.C.

IV. Volume V of the Coblentz Society Infrared Spectra

This volume is now available (see enclosed description). Many spectra from grating spectrometers are included; all spectra are evaluated for quality and usefulness.

The Coblentz Society Newsletter is published at Midland, Michigan. Editor is A. Lee Smith, c/o Dow Corning Corporation, Midland, Michigan 48640.

WHERE DO WE GO FROM HERE WITH GROUP FREQUENCIES?

by N. B. Colthup

Group frequency studies are now becoming more sophisticated in that they are being more closely related to theoretical studies. Whenever a new group frequency turns up in a study of the spectra of related compounds, an effort is immediately made to fully understand the nature of the normal mode of vibration involved. Such tools as polarized infrared, gas contours, selection rules, temperature studies, and the Raman spectrum can be utilized to help in this. Only then will one appreciate the value of this particular group frequency. This is particularly true for the poorer group frequencies such as C=S or P=S for example. We feel that more work should be done with single bonds and how they vary with rotational isomerism. Also, we feel that a good group frequency analysis should include a survey of all the bands of the group, correlatable or not. For example, not only the double bonds should be pinpointed, but a survey of the general type of single bond bands expected for a compound should be done as well.

While certain group frequencies such as trans and vinylidine CH wag or C=O and P=O stretch are insensitive for the most part to mechanical interaction effects, other groups such as cis CH wag C=S, C-Cl, various C-O groups and aromatic CH wag in nitro aromatics are sensitive to mechanical interaction effects. A good understanding of the nature of these effects can greatly improve one's general ability to interpret spectra.